Leading logarithmic contribution to the second-order Lamb shift induced by the loop-after-loop diagram

Vladimir A. Yerokhin

Department of Physics, St. Petersburg State University, Oulianovskaya 1, Petrodvorets, St. Petersburg 198904, Russia

and Institute for High Performance Computing and Data Bases, Fontanka 118, St. Petersburg 198005, Russia

Contribution of order $\alpha^2(Z\alpha)^6\ln^3(Z\alpha)^{-2}$ to the ground-state Lamb shift in hydrogen induced by the loop-after-loop diagram is evaluated analytically. An additional contribution of this order is found compared to the previous calculation by Karshenboim [JETP 76, 541 (1993)]. As a result, an agreement is achieved for this correction between different numerical and analytical methods.

In the present work a part of the two-loop self-energy correction to the Lamb shift in hydrogen is investigated, which is induced by the irreducible part of the diagram in Fig. 1(a). It is referred to as the *loop-after-loop* contribution. The second-order self-energy correction is important for the comparison of the theoretical prediction with the experimental results for the Lamb shift in hydrogen [1] and He^+ [2] and, therefore, it influences the charge radius of the proton which can be extracted from the Lamb shift in hydrogen [3].

The loop-after-loop contribution has been the subject of a recent debate in the literature. Analytic calculations of its $Z\alpha$-expansion coefficients have been carried out by Eides and co-workers [4] and Pachucki [5] in order $\alpha^2(Z\alpha)^5$ and by Karshenboim [6][1] in order $\alpha^2(Z\alpha)^6\ln^3(Z\alpha)^{-2}$. A direct numerical calculation of this correction to all orders in $Z\alpha$ in the low-Z region was reported by Mallampalli and Sapirstein [8]. A fit to the data in Ref. [8] is consistent with the analytical result in order $\alpha^2(Z\alpha)^5$ but it is in significant dis-

[1]The same result was re-derived recently in Ref. [7]

agreement with Karshenboim's calculation of the leading logarithmic contribution. As a consequence, a question was raised in Ref. [8] about the breakdown of the $Z\alpha$ expansion for the two-loop self energy even for hydrogen. The subsequent calculation by Goidenko *et al.* [9], also nonperturbative in $Z\alpha$, shows to be compatible with the analytical results. However, my recent nonperturbative (in $Z\alpha$) calculation [10] exhibits a good agreement with the results of Ref. [8] and yields a corresponding logarithmic contribution which is roughly three times larger than Karshenboim's result. On the contrary, a recent evaluation by Manohar and Stewart [11] supports Karshenboim's value of the leading logarithmic correction for the total two-loop self energy.

In Refs. [6,7] it is argued that the leading logarithmic correction for the two-loop self energy is induced only by the diagram shown in Fig. 2(b), if working in the Fried-Yennie gauge. The numerical calculation of Ref. [10] confirms their value of the corresponding contribution from the diagram in Fig. 2(b). However, it shows also an additional logarithm cubed with a coefficient $a_{63} = -0.652(30)$ originating from the diagram presented in Fig. 2(a). In the present investigation, I derive the leading logarithmic contribution induced by this diagram in the case of the ground state of hydrogenlike ions. The resulting coefficient is found to be $a_{63} = -2/3$, in agreement with my previous numerical result.

The contribution of the loop-after-loop diagram [Fig. 1(a)] can be written as [2]

$$\Delta E_{\rm lal} = \frac{1}{(2\pi)^{12}} \int d\mathbf{p} d\mathbf{k} d\mathbf{k}' d\mathbf{p}' \overline{\psi}_a(\mathbf{p}) \Sigma_R(\mathrm{p},\mathrm{k}) G_a^{\rm red}(\mathrm{k},\mathrm{k}') \Sigma_R(\mathrm{k}',\mathrm{p}') \psi_a(\mathbf{p}') \;, \tag{1}$$

where ψ_a is the ground-state wave function, Σ_R is the renormalized self-energy operator, $G_a^{\rm red}$ is the reduced Coulomb Green function, and the time component of all 4-vectors equals to the ground-state energy ε_a. This expression is not completely gauge invariant, but it can be shown to be gauge independent over covariant gauges. In the present investigation

---

[2]Relativistic units are used in this Letter ($\hbar = c = m = 1$). I use roman style (p) for 4-vectors, bold face ($\mathbf{p}$) for 3-vectors and italic style (p) for scalars. 4-vectors have the form $\mathrm{p} = (\mathrm{p}_0, \mathbf{p})$. The length of the 3-vector $\mathbf{p}$ is denoted by p. I also use the notations $\not{\mathrm{p}} = \mathrm{p}_\mu \gamma^\mu$, $\hat{\mathbf{p}} = \mathbf{p}/|\mathbf{p}|$.

the consideration will be given in the Fried-Yennie gauge. Because of lack of a convenient representation of the Coulomb Green function, the standard way to evaluate Eq. (1) is to expand the inner electron propagators in terms of an interaction with the external nuclear field. Some of the terms of this expansion are shown in Figs. 2[(a),(b)].

The leading contribution to $\Delta E_{\rm lal}$ is of order $\alpha^2(Z\alpha)^5$ and originates from the diagram in Fig. 2(a). It was evaluated in Refs. [4,5] after proving that only relativistic values of the intermediate momentum are responsible for this correction and that both external momenta can be put on the mass shell with vanishing space components. The next-to-leading contribution contains a logarithm cubed. It was derived in Refs. [6,7] by using an effective-potential approach, where the self-energy operator is replaced by a potential on the mass shell,

$$\Sigma_R(\mathrm{p},\mathrm{k}) \to V_{\rm SE} = -\frac{8\alpha(Z\alpha)}{3}\ln k \ . \tag{2}$$

The effective quasilocal potential $V_{\rm SE}$ is defined in a way to generate the leading contribution to the one-loop Lamb shift. Obviously, this potential leads to a squared logarithmic contribution in Eq. (1), after the integration over the intermediate momentum is carried out within the logarithmic region $Z\alpha \ll k \ll 1$. One can gain one more logarithm if $\ln^2 k$ is integrated with a factor $1/k$,

$$\int_{Z\alpha}^1 dk \frac{\ln^2 k}{k} \sim \ln^3 Z\alpha \ . \tag{3}$$

In Refs. [6,7], the factor $1/k$ arises from the second term of the potential expansion of $G_a^{\rm red}$ in Eq. (1). This is the reason why in these considerations Fig. 2(b) yields a logarithm cubed and Fig. 2(a) does not. As we will see below, the treatment of Refs. [6,7] is incomplete. A more accurate investigation shows that an analogous factor $1/k$ can be obtained by taking into account the momentum distribution of the external wave functions in the diagram in Fig. 2(a).

Let us now derive the next-to-leading contribution to the diagram in Fig. 2(a). While its leading term can be evaluated assuming the external momenta being put on the mass shell

with vanishing space components, we intend to keep the first-order terms in the expansion over the space components. The binding energy is still neglected; one can show that it does not contribute to the order of interest. We write the contribution of the diagram in Fig. 2(a) as

$$\Delta E_{2a} = \frac{1}{(2\pi)^9} \int d\mathbf{p} d\mathbf{k} d\mathbf{p}' \psi_a^\dagger(\mathbf{p}) V_C(\mathbf{p}-\mathbf{k}) \mathcal{K}(\mathrm{p},\mathrm{k},\mathrm{p}') V_C(\mathbf{k}-\mathbf{p}') \psi_a(\mathbf{p}') \ , \tag{4}$$

where V_C is the Coulomb potential $V_C(\mathbf{q}) = -4\pi Z\alpha/q^2$, and $\mathcal{K}$ is the kernel

$$\mathcal{K}(\mathrm{p},\mathrm{k},\mathrm{p}') = \gamma_0 \Lambda^{\mathrm{FY}}_{R_0}(\mathrm{p},\mathrm{k}) \frac{\not{\mathrm{k}}+1}{\mathrm{k}^2-1} \Lambda^{\mathrm{FY}}_{R_0}(\mathrm{k},\mathrm{p}') \ , \tag{5}$$

with $\Lambda^{\mathrm{FY}}_{R_\mu}$ being the renormalized vertex operator in the Fried-Yennie gauge. For our purposes it is sufficient to keep only the lowest-order term of the $Z\alpha$ expansion of the Dirac wave function

$$\psi_a(\mathbf{p}) = \begin{pmatrix} g_a(p)\chi_{\kappa_a m_a}(\hat{\mathbf{p}}) \\ f_a(p)\chi_{-\kappa_a m_a}(\hat{\mathbf{p}}) \end{pmatrix} \approx \frac{N}{(p^2+(Z\alpha)^2)^2} \begin{pmatrix} \chi_{\kappa_a m_a}(\hat{\mathbf{p}}) \\ (-p/2)\chi_{-\kappa_a m_a}(\hat{\mathbf{p}}) \end{pmatrix} \ , \tag{6}$$

where $N = (2\pi)^{3/2}(32(Z\alpha)^5/\pi)^{1/2}$. In Eq. (6) and in what follows, the sign of the approximate equality ($\approx$) is used when terms irrelevant for the contribution of interest are dropped. Assuming that the external momentum p is close to the mass shell, we can expand the vertex operator over the space components of p

$$\Lambda^{\mathrm{FY}}_{R_0}(\mathrm{p},\mathrm{k}) \approx \Lambda^{(0)}_0(\mathrm{s},\mathrm{k}) + (\boldsymbol{\gamma}\cdot\mathbf{p})\Lambda^{(1)}_0(\mathrm{s},\mathrm{k}) + (\mathbf{p}\cdot\hat{\mathbf{k}})\Lambda^{(2)}_0(\mathrm{s},\mathrm{k}) + p^2\Lambda^{(3)}_0(\mathrm{s},\mathrm{k}) \ , \tag{7}$$

where s is a 4-vector with zero space components, $\mathrm{s} = (1,\mathbf{0})$. The parts of ΔE_{2a} induced by the four terms in the righthand side of Eq. (7) are denoted by ΔE_i, $i = 0\ldots3$.

The correction ΔE_0 can be written by introducing an effective wave function φ_0 as

$$\Delta E_0 = \int \frac{d\mathbf{k}}{(2\pi)^3} \varphi_0^\dagger(\mathbf{k}) \mathcal{K}(\mathrm{s},\mathrm{k},\mathrm{s}) \varphi_0(\mathbf{k}) \ , \tag{8}$$

where

$$\varphi_0(\mathbf{k}) = \int \frac{d\mathbf{p}}{(2\pi)^3} V_C(\mathbf{k}-\mathbf{p}) \psi_a(\mathbf{p}) \approx -\frac{N}{2k^2} \begin{pmatrix} \chi_{\kappa_a m_a}(\hat{\mathbf{k}}) \\ -\dfrac{Z\alpha}{2} \operatorname{arctg}\dfrac{k}{Z\alpha}\, \chi_{-\kappa_a m_a}(\hat{\mathbf{k}}) \end{pmatrix} \ . \tag{9}$$

Eq. (8) contains a contribution of the previous order. To eliminate it, one should subtract the same expression with the Dirac bispinors replaced by the Schrödinger wave functions. This means that we are interested only in the part of Eq. (8) which contains a product of the upper and lower components of φ_0. Considering the matrix structure of the kernel $\mathcal{K}$, one can see that only the part of $\mathcal{K}$ proportional to $\gamma_0(\boldsymbol{\gamma}\cdot\mathbf{k})$ provides a nonzero contribution to the order of interest. Therefore, we have

$$\mathcal{K}(\mathrm{s},\mathrm{p},\mathrm{s}) \approx -\frac{\alpha^2}{(4\pi)^2}\frac{\gamma_0(\boldsymbol{\gamma}\cdot\mathbf{k})}{k^2}\mathcal{F}_0(k)\ . \tag{10}$$

One can show that $\mathcal{F}_0(k) \approx -(112/3)k^2\ln^2 k^2$ for small k. Keeping in mind that logarithms normally arise from integrals like Eq. (3), we can cut off the integration over k in Eq. (8) by an arbitrary constant $\Lambda \sim 1$ and use the low-energy asymptotic form for $\mathcal{F}(k)$,

$$\Delta E_0 \approx -\frac{\alpha^2(Z\alpha)^6}{2\pi^3}\frac{112}{3}\int_0^\Lambda dk\frac{\ln^2 k^2}{k}\,\mathrm{arctg}\frac{k}{Z\alpha}\ . \tag{11}$$

If $Z\alpha$ is set to zero under the integral, it would logarithmically diverge for small values of k. Therefore, $Z\alpha$ can be regarded as an effective cut-off parameter in this case. We can cut off the k-integration by $Z\alpha$ and then set $Z\alpha$ to zero under the integral

$$J \equiv \int_0^\Lambda dk\frac{\ln^2 k^2}{k}\,\mathrm{arctg}\frac{k}{Z\alpha} \approx \frac{\pi}{2}\int_{Z\alpha}^\Lambda dk\frac{\ln^2 k^2}{k} \approx \frac{\pi}{12}\ln^3(Z\alpha)^{-2}\ . \tag{12}$$

A rigorous evaluation of the integral J yields the same value of the cubed logarithmic contribution. So, we have for the correction ΔE_0

$$\Delta E_0 \approx \left(-\frac{14}{9}\right)\frac{\alpha^2}{\pi^2}(Z\alpha)^6\ln^3(Z\alpha)^{-2}\ . \tag{13}$$

The evaluation of the remaining corrections is carried out in a similar way. By a direct calculation one can show that $\Delta E_1 \approx 0$. The correction ΔE_2 is written as

$$\begin{aligned}\Delta E_2 = -\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{k^2}\Big\{&\varphi_2^\dagger(\mathbf{k})\gamma_0\Lambda_0^{(2)}(\mathrm{s},\mathrm{k})(\not{k}+1)\Lambda_0^{(0)}(\mathrm{k},\mathrm{s})\varphi_0(\mathbf{k})\\ &+\varphi_0^\dagger(\mathbf{k})\gamma_0\Lambda_0^{(0)}(\mathrm{s},\mathrm{k})(\not{k}+1)\Lambda_0^{(2)}(\mathrm{k},\mathrm{s})\varphi_2(\mathbf{k})\Big\}\ ,\end{aligned} \tag{14}$$

with a wave function φ_2

$$\varphi_2(\mathbf{k}) = \int \frac{d\mathbf{p}}{(2\pi)^3}(\mathbf{p}\cdot\hat{\mathbf{k}})V_C(\mathbf{k}-\mathbf{p})\psi_a(\mathbf{p})$$
$$\approx -\frac{N}{2k^2}(Z\alpha)\,\mathrm{arctg}\frac{k}{Z\alpha}\begin{pmatrix}\chi_{\kappa_a m_a}(\hat{\mathbf{k}})\\ 0\end{pmatrix}\ . \tag{15}$$

Keeping only terms proportional to the product of the upper components, we have

$$\Delta E_2 \approx -\frac{\alpha^2(Z\alpha)^6}{\pi^3}\int_0^\infty dk\frac{\mathcal{F}_2(k)}{k^4}\,\mathrm{arctg}\frac{k}{Z\alpha}\ , \tag{16}$$

where the function $\mathcal{F}_2(k)$ can be found to have an asymptotic form $\mathcal{F}_2(k) \approx -(64/9)k^3\ln^2 k^2$ for small k. Immediately, we have

$$\Delta E_2 \approx \frac{64}{9}\,\frac{\alpha^2}{\pi^3}(Z\alpha)^6 J \approx \frac{16}{27}\,\frac{\alpha^2}{\pi^2}(Z\alpha)^6\ln^3(Z\alpha)^{-2}\ . \tag{17}$$

The correction ΔE_3 is evaluated in the same way as ΔE_2 by introducing a new wave function φ_3

$$\varphi_3(\mathbf{k}) = \int \frac{d\mathbf{p}}{(2\pi)^3}p^2 V_C(\mathbf{k}-\mathbf{p})\psi_a(\mathbf{p})$$
$$\approx -\frac{N}{k}(Z\alpha)\,\mathrm{arctg}\frac{k}{Z\alpha}\begin{pmatrix}\chi_{\kappa_a m_a}(\hat{\mathbf{k}})\\ 0\end{pmatrix}\ . \tag{18}$$

The derivation yields

$$\Delta E_3 \approx \frac{8}{27}\,\frac{\alpha^2}{\pi^2}(Z\alpha)^6\ln^3(Z\alpha)^{-2}\ . \tag{19}$$

Adding all evaluated corrections, we have for the total cubed logarithmic contribution from the diagram in Fig. 2(a)

$$\Delta E_{2a} \approx \sum_{i=0}^{3}\Delta E_i \approx \left(-\frac{2}{3}\right)\frac{\alpha^2}{\pi^2}(Z\alpha)^6\ln^3(Z\alpha)^{-2}\ . \tag{20}$$

The results are commonly represented in the form of a double expansion over $(Z\alpha)$ and $\ln(Z\alpha)^{-2}$

$$\Delta E = \left(\frac{\alpha}{\pi}\right)^2\sum_{ij}a_{ij}\,(Z\alpha)^i\ln^j(Z\alpha)^{-2}\ . \tag{21}$$

In this notation the leading logarithmic contribution induced by the diagram in Fig. 2(a) is found to be $a_{63} = -2/3$, in a good agreement with $a_{63} = -0.652(30)$ obtained in my previous

calculation [10]. This result, together with the corresponding contribution from the diagram in Fig. 2(b) evaluated in Ref. [6], yields the total correction of order $\alpha^2(Z\alpha)^6\ln^3(Z\alpha)^{-2}$ for the loop-after-loop diagram [Fig. 1(a)], $a_{63} = -2/3 - 8/27 = -26/27 \approx -0.963$. This value is in good agreement with the numerical result of Mallampalli and Sapirstein $a_{63} = -0.9$ [8] and with my numerical calculation $a_{63} = -1.01(8)$ [10]. However, it strongly disagrees with the evaluation by Goidenko and co-workers [9]. A possible reason for this discrepancy may be a non-covariant renormalization procedure used in that work, which is known to provide spurious contributions in some cases. This topic is discussed in more detail in Ref. [10].

In the present work, only the irreducible part of the diagram in Fig. 1(a) is investigated. The question if the remaining two diagrams of the two-loop self energy provide a cubed logarithmic contribution, remains still unclear. An indication that it could be the case are the results of Pachucki [12] and Manohar and Stewart [11]. The authors calculated the leading logarithmic contribution to the total two-loop self energy by working in Coulomb gauge [12] and within the renormalization-group approach [11]. Both evaluations agree with Karshenboim's result. Keeping in mind that we derived the additional contribution from the diagram Fig. 1(a), one should deduce that the remaining diagrams Figs. 1[(b),(c)] provide the same contribution with the opposite sign, if working in a covariant gauge.

In summary, I derived an additional cubed logarithmic contribution to the loop-after-loop correction for the ground state of hydrogenlike ions. As a result, an agreement between the results of numerical and analytical methods is achieved. Therefore, there are no grounds at present to question the validity of the $Z\alpha$ expansion for hydrogen. However, the convergence of this expansion for the two-loop self energy is remarkably slow. As was shown in Ref. [10], the first three expansion terms for the loop-after-loop correction cover only about 50% of the total result for hydrogen. Thus, it is highly desirable to carry out exact calculations of the remaining part of the two-loop self energy in the low-Z region.

I would like to thank Prof. Shabaev for his guidance and continued interest during the course of this work. Valuable conversations with S. G. Karshenboim are gratefully acknowledged. I thank also M. I. Eides, L. N. Labzowsky, and Th. Beier for interesting discussions.

This work was supported in part by the Russian Foundation for Basic Research (Grant No. 98-02-18350) and by the program "Russian Universities. Basic Research" (project No. 3930).

---

[1] M. Niering, R. Holzwarth, J. Reichert, P. Pokasov, Th. Udem, M. Weitz, T. W. Hänsch, P. Lemonde, G. Santarelli, M. Abgrall, P. Laurent, C. Salomon, and A. Clairon, Phys. Rev. Lett. **84**, 5496 (2000).

[2] A. van Wijngaarden, J. Kwela, and G. W. F. Drake, Phys. Rev. A **43**, 3325 (1991).

[3] S. G. Karshenboim, Can. J. Phys. **77**, 241 (1999).

[4] M. I. Eides, S. G. Karshenboim, and V. A. Shelyuto, Phys. Lett. B **312**, 358 (1993); Physics of Atomic Nuclei **57**, 1240 (1994).

[5] K. Pachucki, Phys. Rev. Lett. **72**, 3154 (1994).

[6] S. G. Karshenboim, Zh. Eksp. Teor. Fiz. **103**, 1105 (1993) [Sov. Phys. JETP **76**, 541 (1993)].

[7] M. I. Eides, H. Grotch, and V. A. Shelyuto, *Theory of light hydrogenlike ions.*, hep-ph/0002158, 15 February 2000.

[8] S. Mallampalli and J. Sapirstein, Phys. Rev. Lett. **80**, 5297 (1998).

[9] I. Goidenko, L. Labzowsky, A. Nefiodov, G. Plunien, and G. Soff, Phys. Rev. Lett **83**, 2312 (1999).

[10] V. A. Yerokhin, Phys. Rev. A **62**, 012508 (2000).

[11] A. V. Manohar and I. V. Stewart, Phys. Rev. Lett. **85**, 2248 (2000).

[12] K. Pachucki, private communication.

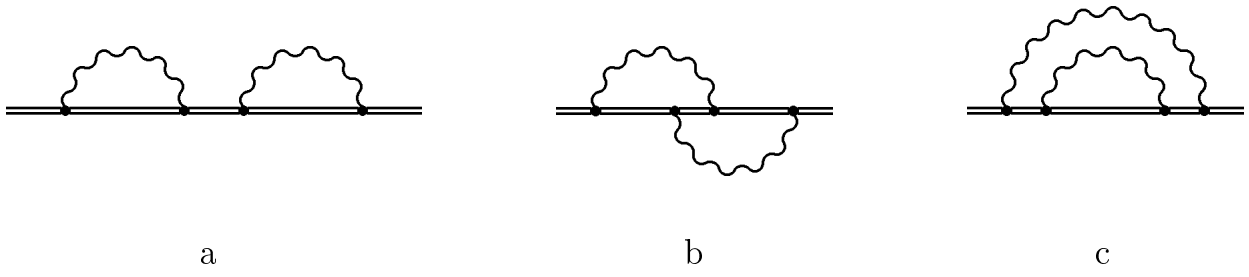

FIG. 1. One-electron self-energy Feynman diagrams of second order in α.

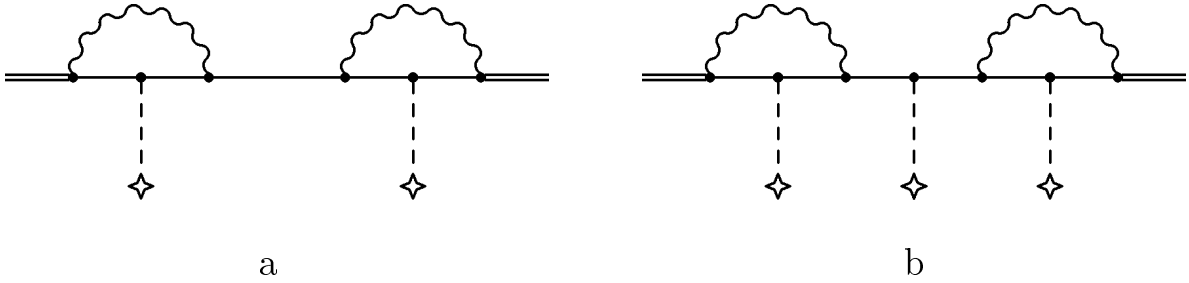

FIG. 2. Two terms of the potential expansion of the diagram in Fig. 1(a). A double line denotes an electron in the field of the nucleus. A single line indicates a free electron. A dashed line denotes a Coulomb interaction with the nucleus.